The ATOMIC Equation of State

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We report on meeting a major deliverable for the development of ATOMIC, a code designed to compute opacities under both local thermodynamic equilibrium (LTE) and non-LTE conditions for a large range of elements. ATOMIC will become the successor of the T-4 opacity code LEDCOP. The calculations shown here demonstrate that all the equation of state (EOS) capabilities have been successfully implemented into ATOMIC and are robust enough to calculate opacity tables over a wide range of temperatures and densities and for various atomic systems.

The basis of ATOMIC is the FORTRAN 90 reconstruction of the FINE nonequilibrium spectral modeling code, to which physics packages extracted from LEDCOP have been added. ATOMIC provides improved atomic physics data, a user-friendly interface, modularity to facilitate code improvements, platform independence, and less manipulation of the atomic physics databases than is currently necessary for LEDCOP. The development of ATOMIC in FORTRAN 90 also provides a platform for parallelization of both the LTE and non-LTE calculations.

A complete opacity table contains on average about 2,000 density-temperature points. To keep the production time tractable, we developed a parallel scheme where density-temperature point calculations are distributed over the set of processors used in the calculation. The parallel scheme makes use of a simple queuing system where the next density-temperature point is sent to the first processor that has completed the calculation at a previously given condition. This scheme allows for an efficient use of the parallel resource and its performance is independent of the number of processors used.

ATOMIC makes use of a new model to calculate the EOS. The model is based on the chemical picture, which aims at minimizing the Helmholtz free energy. The plasma is represented as an ensemble of various species corresponding to the electrons and the different ion stages. Plasma and density effects are included within the framework of the occupation probability formalism as developed by Mihalas and coworkers [1, 2]. A package has been developed, implemented in ATOMIC, and tested for hydrogen, helium, and oxygen over the whole density-temperature conditions needed for the production of an opacity table.

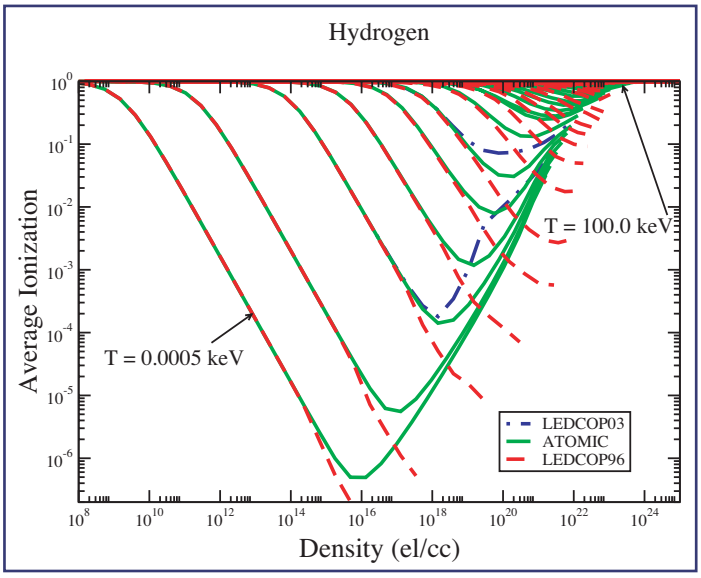

Figure 1—
Hydrogen ionization fraction calculated by ATOMIC and LEDCOP.

Figure 1 shows a comparison of the hydrogen effective ionization fraction, Z, calculated with ATOMIC and LEDCOP. Figure 1 shows a significant improvement for the calculation of the hydrogen EOS, particularly in the region where pressure ionization is important, i.e., for electron densities greater than 10^{20} elec./cm^3. One sees in Fig. 1 that the EOS implemented in LEDCOP tends to fail dramatically when pressure ionization becomes important. In contrast, the new EOS provides a smooth transition along each isotherm when density effects lead to an increase in the ionization fraction.

This result indicates that the new EOS developed for ATOMIC will allow to extend current opacity tables to higher densities.

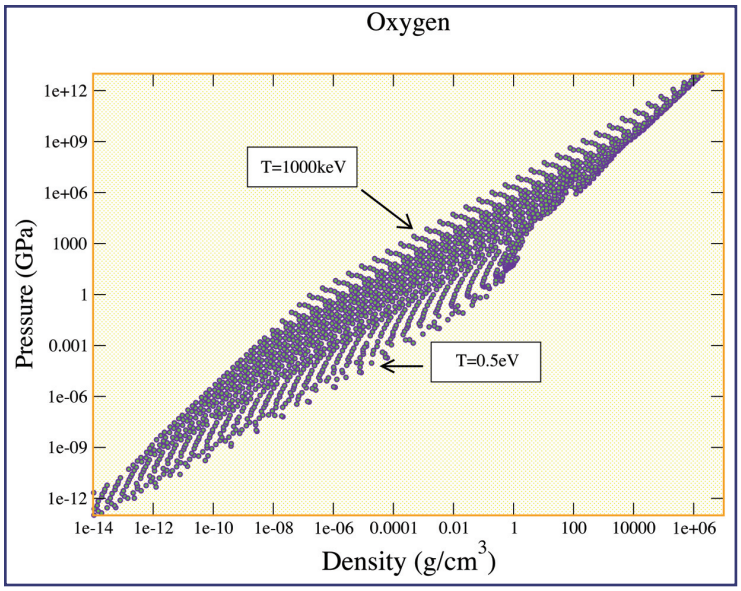

Figure 2— Variation of the oxygen pressure as a function of density and temperature.

The calculation of the EOS for a more complicated system such as oxygen is not straightforward in the current formalism as the number of ion stages of the species under consideration translates into an equivalent number of coupled nonlinear equations to be solved. In addition, the various density and plasma terms entering the set of nonlinear equations vary rather drastically as a function of density and, as such, the number of nonlinear equations to be solved also varies along a given isotherm. To keep the calculation time sufficiently low to enable the production of a complete opacity table and independent of the species involved, we developed a computational scheme that only uses a restricted number of ion stages. The ion stages needed at a given density-temperature condition are selected by first finding the four ion stages that minimize the free energy using the average configuration properties. This calculation is followed by a second minimization of the free energy where two additional ion stages are included and, this time, using the fine structure level properties. This scheme has been implemented and tested for oxygen for the whole density-temperature conditions needed for the production of an opacity table. Figure 2 shows the result of this calculation for the oxygen pressure and along the complete opacity table.

In conclusion, we have developed, tested, and implemented in ATOMIC a new scheme to calculate the EOS. This new model indicates that the physics models included provide a better description of the density and plasma effects than in the previous opacity code LEDCOP. We have also demonstrated that the model implemented is also efficient to calculate the EOS of more complex systems by calculating the oxygen EOS for all the density-temperature conditions needed for an opacity table production. Finally, as the computational scheme implemented only uses a fixed number of ion stages, we anticipate that the model implemented can be readily applied to elements with higher atomic number without a significant increase in computational time.

[1] W. Dappen, L. Anderson, and D. Mihalas, *Ap. J.* **319**, 195 (1987).
[2] D. Saumon and G. Chabrier, *Phys. Rev A* **44**, 5122 (1991).

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